SIAM J. OPTIM.
Vol. 9, No. 1, pp. 53–61
© 1998 Society for Industrial and Applied Mathematics

STOCHASTIC SIMULATION ON INTEGER CONSTRAINT SETS*

I. H. DINWOODIE†

Abstract. Bounds are given on the number of steps sufficient for convergence of simulation algorithms on domains of nonnegative integer constraint sets.

Key words. Markov chains, eigenvalues, annealing, integer optimization

AMS subject classifications. 60J20, 65K05, 90C10

PII. S1052623496313842

1. Introduction.

This article is concerned with convergence of Markov chains on nonnegative integer constraint sets and applications to simulated annealing algorithms for optimization.

Despite the lack of applicable results on its performance, the annealing algorithm is used for optimization of nonlinear functions on discrete domains. One application of the algorithm is finding modes of probability distributions on finite sets, a problem which arises in Bayesian statistics and image analysis (see [6] and [14]). It is used for other problems in combinatorial optimization as well, some of which are described in [13]. Here we are interested in domains of nonnegative integer lattice points on hyperplanes, which arise in integer optimization problems, image analysis, and statistics. Symmetric Markov chains on these domains were constructed in [4] using algebraic techniques.

Whereas optimal cooling schedules have been widely studied [1], [7], [8], [9], we are interested in establishing clear bounds on the time required for a given accuracy $\delta > 0$ and reliability $\varepsilon > 0$. The main result is Theorem 3.1, which gives a sufficient number of steps in the algorithm in a computable form. We expect that the results can be improved as new technology in Markov chains becomes available. They are based on geometrical techniques from [3] and [9], which also are used in the more general and abstract study [10].

Let us establish some notation. Let $\mu > 0$ be a probability distribution function on the set $S = \{\mathbf{x} \in Z_+^d, A(\mathbf{x}) = \mathbf{b} \in Z_+^r\}$, where A is a linear map or matrix with nonnegative integer entries such that S is finite. We show first in section 2 how to simulate from μ using techniques from [4], then we get convergence rates from eigenvalue estimates and apply these results in section 3 to the case where μ is chosen to put most of its mass where f is small. Our Markov chain is homogeneous, which means that the parameter β corresponding to the reciprocal of temperature is held fixed over time at a level which gives the desired stationary distribution.

2. The algorithm.

We define a symmetric Markov chain on S as follows. Let $Q(\xi_1, \ldots, \xi_d)$ be the ring of polynomials in variables $\xi_1, \ldots, \xi_d$ with coefficients in the rational numbers Q. If $\mathbf{x}$ is a vector of nonnegative integers, define $X^{\mathbf{x}} = \xi_1^{x_1} \cdots \xi_d^{x_d}$.

Let $M = \{g_1, \ldots, g_m\}$, where $g_i \in Z^d$ and $\{X^{g_i^+} - X^{g_i^-} : i = 1, \ldots, m\}$ is a Gröbner basis for the ideal I_A in $Q(\xi_1, \ldots, \xi_d)$ given by $I_A = \langle X^{\mathbf{v}} - X^{\mathbf{w}} : A(\mathbf{v}) =$

*Received by the editors December 18, 1996; accepted for publication (in revised form) January 5, 1998; published electronically October 30, 1998.
http://www.siam.org/journals/siopt/9-1/31384.html
†Department of Mathematics, Tulane University, New Orleans, LA 70118 (ihd@math.tulane.edu).

$A(\mathbf{w})\rangle$. Recall that $g = g^+ - g^-$, where $g^+ = \max\{g, 0\}$, $g^- = \max\{-g, 0\}$. Our ordering on monomials is purely lexicographic, based on the indeterminate ordering $\xi_1 > \xi_2 > \cdots > \xi_d$.

Now define a Markov chain on S as follows. Let $\mathbf{x} = (x_1, \ldots, x_d)$ denote an element of S, and let $N_{\mathbf{x}}$ be the set of its neighbors in S, so $N_{\mathbf{x}} = \{\mathbf{x} \pm g_i : \mathbf{x} \pm g_i \geq 0, g_i \in M\}$. Let $K(\mathbf{x}, \cdot)$ be the probability vector

$$K(\mathbf{x}, \mathbf{y}) = \frac{1}{2m} \qquad \text{for } \mathbf{y} \in N_{\mathbf{x}}.$$

Also, $K(\mathbf{x}, \mathbf{x}) = 1 - \sum_{\mathbf{y} \in N_{\mathbf{x}}} K(\mathbf{x}, \mathbf{y})$ makes the vector sum to 1 and will be positive precisely when $|N_{\mathbf{x}}| < 2m$. The transition can be realized by uniformly choosing an element $\pm g_i$ from among the $2m$ choices $\{\pm g_1, \ldots, \pm g_m\}$ and adding it to $\mathbf{x}$ if the result is nonnegative. Then K is symmetric, irreducible, and aperiodic.

Recall that $\mu > 0$ is an arbitrary distribution on S. Let K_μ be the transition matrix given by

$$K_\mu(\mathbf{x}, \mathbf{y}) = K(\mathbf{x}, \mathbf{y}) \min\{\mu(\mathbf{y})/\mu(\mathbf{x}), 1\}, \qquad \mathbf{x} \neq \mathbf{y},$$

and the holding probability makes the matrix stochastic. Let the spectrum of K_μ be $1 = \lambda_1 > \lambda_2 \geq \cdots \geq \lambda_{|S|} > -1$, and let $\gamma = 1 - \lambda_2$. In the next section, μ will depend on a parameter $\beta > 0$ interpreted as the reciprocal of temperature.

To estimate γ, observe that

$$\begin{aligned}
\gamma &= \inf_{\phi} \frac{\langle \phi, (I - K_\mu)\phi \rangle_\mu}{\|\phi - \langle \phi, \mathbf{1} \rangle_\mu \mathbf{1}\|_\mu^2} \\
&= \inf_{\phi} \frac{\sum_{(x,y)} (\phi(x) - \phi(y))^2 \mu(x) K_\mu(x, y)}{\sum_{(x,y)} (\phi(x) - \phi(y))^2 \mu(x) \mu(y)} \\
&= \inf_{\phi} \frac{\sum_{e \in G} \phi(e)^2 Q(e)}{\sum_{f \in G_c} \phi(f)^2 Q_c(f)},
\end{aligned}$$

where ϕ ranges through nonconstant functions on the state space S, G is the graph with edge $e = \{x, y\}$ if and only if $Q(e) = \mu(x)K_\mu(x, y)$ $(= \mu(y)K_\mu(y, x)) > 0$, and G_c is the complete graph with edges $f = \{x, y\}$ connecting all ordered pairs, $Q_c(f) = \mu(x)\mu(y)$, and $\phi(f)^2 = (\phi(y) - \phi(x))^2$. Now this representation can be used as in [3] and [9] to bound $1/\gamma$ from above in the form of a Poincaré inequality, which we use in Lemma 2.1 below.

Define the following quantities. Let $\mu_{\max} = \max\{\mu(\mathbf{x})\}$, $\mu_{\min} = \min\{\mu(\mathbf{x})\}$, $\rho = \mu_{\max}/\mu_{\min}$. The following eigenvalue estimate uses a result of [3], which is implicit in [9]. Recall that m is the number of moves in the set M.

LEMMA 2.1. *Let $\gamma = 1 - \lambda_2$. Then $1/\gamma \leq m\rho\mu_{\max}|S|^3$.*

Proof. If $\mathbf{x} > \mathbf{y}$ are two points in S ordered lexicographically, form a path from $\mathbf{x}$ to $\mathbf{y}$ by dividing the monomial difference $X^{\mathbf{x}} - X^{\mathbf{y}}$ by the Gröbner basis $\{X^{g_i^+} - X^{g_i^-} : 1 \leq i \leq m\}$, ordered in some arbitrary but fixed way. The multidegrees of the lead terms in the division give a path $p_{\mathbf{xy}}$ which joins the endpoints $\mathbf{x}$ and $\mathbf{y}$ with decreasing (in lexicographic order) path segments to a common point in S. The number of edges in this path $p_{\mathbf{xy}}$ is no greater than $\#\mathbf{x} - 1$, if $\#\mathbf{x}$ is the rank of $\mathbf{x}$ in the set S using

lexicographic order (the smallest element of S in lexicographic order has rank 1, the largest has rank $|S|$). Define the measure of length $|p_{\mathbf{xy}}|_Q = \sum_{e\in p_{\mathbf{xy}}} Q(e)^{-1}$.

Proposition 1 of [3] shows that $1/\gamma \le \max_e \sum_{p_{\mathbf{xy}}\ni e} |p_{\mathbf{xy}}|_Q\, \mu(\mathbf{x})\mu(\mathbf{y})$, where $p_{\mathbf{xy}}$ is the path from $\mathbf{x}$ to $\mathbf{y}$ constructed above and e is an edge in the graph on S, say $\{\mathbf{a}, \mathbf{a}\pm g_\alpha\}$, with $Q(e) = \mu(\mathbf{a})K_\mu(\mathbf{a}, \mathbf{a}\pm g_\alpha) = \mu(\mathbf{a})K(\mathbf{a}, \mathbf{a}\pm g_\alpha)\min\{\mu(\mathbf{a}\pm g_\alpha)/\mu(\mathbf{a}), 1\}$. Then $Q(e)^{-1} \le \mu_{\min}^{-1}(2m)$.

For $\mathbf{x}\in S$, the maximum number of edges in a path joining $\mathbf{x}$ to $\mathbf{y} < \mathbf{x}$ is $\#\mathbf{x} - 1$, so $|p_{\mathbf{xy}}|_Q \le (\#\mathbf{x} - 1)2m/\mu_{\min}$. With $e = \{\mathbf{a}, \mathbf{a} - g_\alpha\}$, the paths through e can be partitioned into collections starting at the different maximal values $\mathbf{x} \ge \mathbf{a}$. There can be at most $\#\mathbf{x} - 1$ paths starting from $\mathbf{x} \ge \mathbf{a}$ and going to some point less than $\mathbf{x}$, and the length of each is at most $\#\mathbf{x} - 1$. Thus

$$\begin{aligned}\sum_{p_{\mathbf{xy}}\ni e} |p_{\mathbf{xy}}|_Q\, \mu(\mathbf{x})\mu(\mathbf{y}) &\le 2m/\mu_{\min} \sum_{\mathbf{x}\ge\mathbf{a}} (\#\mathbf{x} - 1)^2 {\mu^2}_{\max} \\ &\le 2m\left({\mu^2}_{\max}/\mu_{\min}\right) \sum_{\mathbf{x}} (\#\mathbf{x} - 1)^2 \\ &= 2m\left({\mu^2}_{\max}/\mu_{\min}\right)(|S| - 1)|S|(2|S| - 1)/6 \\ &\le m\rho\mu_{\max}|S|^3. \qquad \square\end{aligned}$$

The main contribution of the bound in Lemma 2.1 is the estimate for γ when μ is uniform. Since the paths in the estimate joining two points do not change with μ, they cannot yield the optimal result for a particular μ (see [9]). On the other hand, the technique gives a practical estimate of the path length $|p_{\mathbf{xy}}|_Q$. In some examples, one can find a shorter path by going through intermediate points and using various orderings on the variables $\xi_1, \ldots, \xi_d$ for different path segments. This applies in particular to Example 3.3.

Finally let T_μ be the Markov chain obtained by running K_μ a Poisson(1) number of steps each time to avoid complications from negative eigenvalues. If we let $\Delta = K_\mu - I$ be the generator for K_μ, we can define

$$T_\mu = e^{\Delta}, \tag{2.1}$$

which is reversible with stationary distribution μ. The spectrum of e^Δ is $\{\exp(\lambda_i - 1), i = 1, \ldots, |S|\}$.

Recall that any reversible and irreducible kernel T with stationary distribution $\mu > 0$ implies that multiplying the matrix T with a column vector on the right gives a self-adjoint operator on $L^2(\mu)$, which leaves invariant $\mathbf{1}^\perp$, and multiplying T with a row vector on the left gives a self-adjoint operator on $L^2(1/\mu)$, which leaves invariant $\mu^\perp$. If $\langle\cdot,\cdot\rangle_{1/\mu}$ denotes the inner product in $L^2(1/\mu)$,

$$\begin{aligned}|T^n(\mathbf{x}, A) - \mu(A)| &= \langle(\delta_{\mathbf{x}} - \mu)T^n, (I_A - \mu(A))\mu\rangle_{1/\mu} \\ &\le \|\delta_{\mathbf{x}} - \mu\|_{1/\mu}\|T^n\|_{1/\mu}\|(I_A - \mu(A))\mu\|_{1/\mu}\end{aligned}$$

and $\|\delta_{\mathbf{x}} - \mu\|_{1/\mu} \le 1/\sqrt{\mu(\mathbf{x})}$, $\|(I_A - \mu(A))\mu\|_{1/\mu} \le 1/2$, $\|T^n\|_{1/\mu}$ is its largest eigenvalue as an operator restricted to $\mu^\perp$, which in our situation is $\exp(-\gamma)$.

For two distributions μ and ν on S, define the total variation distance $\|\nu - \mu\| = \sup_{A\subset S} |\nu(A) - \mu(A)|$.

PROPOSITION 2.1. *Let $\varepsilon > 0$, and let T_μ be defined in* (2.1). *Then $\|T_\mu^n(\mathbf{x}, \cdot) - \mu\| \le \varepsilon$ for all $n \ge -m\rho\mu_{\max}|S|^3 \log(\varepsilon\sqrt{\mu(\mathbf{x})})$.*

Proof. Since $\|T_\mu^n(\mathbf{x}, \cdot) - \mu\| \le 1/\sqrt{\mu(\mathbf{x})}\, \exp(-n\gamma)$ (see [3]), it is sufficient that $n \ge -\log(\varepsilon\sqrt{\mu(\mathbf{x})})/\gamma$, which follows if $n \ge -\log(\varepsilon\sqrt{\mu(\mathbf{x})})(m\rho\mu_{\max}|S|^3)$. $\square$

3. Application to simulated annealing. Let $f : S \to \mathbf{R}$, and let $f_{\min} = \min\{f(\mathbf{x}) : \mathbf{x} \in S\} = f(\mathbf{x}_*)$, $f_{\max} = \max\{f(\mathbf{x}) : \mathbf{x} \in S\}$, and set $h = f_{\max} - f_{\min}$. Our optimization problem is to minimize f. Let μ_β be the Gibbs measure on S given by $\mu_\beta(\mathbf{x}) = e^{-\beta f(\mathbf{x})}|S|^{-1}/\phi(-\beta)$, where ϕ is the moment generating function for f with respect to the uniform distribution on S:

$$\phi(t) = \sum_{\mathbf{x}} \frac{e^{tf(\mathbf{x})}}{|S|}. \tag{3.1}$$

Also, let $\phi_\beta(t) = E_\beta e^{tf} = \phi(t-\beta)/\phi(-\beta)$. Let $(\log\phi)^*$ denote the convex conjugate of the function $\log(\phi)$, given by $(\log\phi)^*(a) = \sup_{t\in\mathbf{R}}\{ta - \log\phi(t)\}$. Recall that μ_β converges, as β gets large, to the uniform distribution on the points where f attains its minimum, which we make precise in Lemma 3.1 below.

LEMMA 3.1. *Let $\delta > 0$, let $\varepsilon > 0$, and set $a = f_{\min} + \delta$. Let $\beta > 0$ be sufficiently large that both $E_\beta(f) < a$ and $a(-\beta) - \log\phi(-\beta) \le \log(\varepsilon) + (\log\phi)^*(a)$. Then $\mu_\beta(\{\mathbf{x} : f(\mathbf{x}) > a\}) \le \varepsilon$.*

Proof. Clearly $\mu_\beta(\{\mathbf{x} : f(\mathbf{x}) > a\}) \le e^{-ta}E_\beta e^{tf} = e^{-ta}\phi_\beta(t)$ for all $t \ge 0$, so

$$\begin{aligned}
\log\mu_\beta(\{\mathbf{x} : f(\mathbf{x}) > a\}) &\le -\sup_{t\ge 0}\{ta - \log\phi_\beta(t)\} \\
&= -\sup_{t\in\mathbf{R}}\{ta - \log\phi_\beta(t)\} \qquad \text{(since } a > E_\beta(f)\text{)} \\
&= -\sup_{t}\{(t-\beta)a - \log\phi(t-\beta)\} - a\beta - \log\phi(-\beta) \\
&= -(\log\phi)^*(a) - \beta a - \log\phi(-\beta).
\end{aligned}$$

Let $\beta > 0$ be sufficiently large that $E_\beta(f) < a$ and $a(-\beta) - \log\phi(-\beta) \le \log(\varepsilon) + (\log\phi)^*(a)$. Then the result follows. □

Let $\mathbf{x} = X_0, X_1, \ldots$ be the Markov chain defined in (2.1) with stationary distribution μ_β, transition matrix $T_\beta = e^\Delta$ with $\Delta = I - K_\beta$, and probability measure $P^\beta_{\mathbf{x}}$ on the sample space. Note that $\max\{\mu_\beta(\mathbf{x})\} = \mu_\beta(\mathbf{x}_*) = \mu_{\beta,\max}$.

THEOREM 3.1. *Let $a = f_{\min} + \delta$ for $\delta > 0$, and let $\beta > 0$ be sufficiently large that $E_\beta(f) < a$ and $a(-\beta) - \log\phi(-\beta) \le \log(\varepsilon) + (\log\phi)^*(a)$. Then $P^\beta_{\mathbf{x}}\{f(X_n) > a\} \le 2\varepsilon$ for all $n \ge -m\mu_{\beta,\max}e^{\beta h}|S|^3\log(\varepsilon\sqrt{\mu_\beta(\mathbf{x})})$.*

Remark. For the uniform distribution, the result simplifies to

$$n \ge -m|S|^2\log(\varepsilon/\sqrt{|S|}).$$

Proof. First,

$$\begin{aligned}
P^\beta_{\mathbf{x}}\{f(X_n) > a\} &= P^\beta_{\mathbf{x}}\{X_n \in f^{-1}(a,\infty)\} - \mu_\beta(f^{-1}(a,\infty)) + \mu_\beta(f^{-1}(a,\infty)) \\
&\le \|T^n_\beta(\mathbf{x},\cdot) - \mu_\beta\| + \mu_\beta(f^{-1}(a,\infty)).
\end{aligned}$$

By Proposition 2.1, $\|T^n_\beta(\mathbf{x},\cdot) - \mu_\beta\| \le \varepsilon$ if $n \ge -m\mu_{\beta,\max}e^{\beta h}|S|^3\log(\varepsilon\sqrt{\mu_\beta(\mathbf{x})})$, since the parameter $\rho = \max\{\mu_\beta\}/\min\{\mu_\beta\} = \exp(\beta(f_{\max} - f_{\min})) = \exp(\beta h)$. In addition, $\mu_\beta(f^{-1}(a,\infty)) \le \varepsilon$ if β is sufficiently large (depending on δ and ε) by Lemma 3.1. □

Theorem 3.1 suggests the following. If $\varepsilon = 1/2$ and the Markov chain starts at a point $\mathbf{x}$ not far from $\mathbf{x}_*$ so that $\mu_\beta(\mathbf{x}) \approx \mu_\beta(\mathbf{x}_*) \approx 1$, then a sufficient number of iterations is roughly $me^{\beta h}|S|^3$. This does not give the exact exponential rate of

growth in β of [9], but the bound leaves no unspecified constants and does not rely on detailed knowledge of the function f.

It may be simpler and faster to get the same reliability by running several independent chains with moderate values of β and observing the minimum over all these chains.

EXAMPLE 3.1. *Let* $S = \{\mathbf{x} \in Z_+^2 : x_1 + x_2 = k - 1\}$ *for an integer* $k > 0$. *Then* $|S| = k$. *Let* $\beta = 0$, *which corresponds to infinite temperature. Then* μ_β *is the uniform distribution on* $S = \{(0, k-1), \ldots, (k-1, 0)\}$. *A Gröbner basis consists of the difference* $x_1 - x_2$ *which corresponds to the vector* $g_1 = (1, -1)$, *and the Markov chain* K_0 *is essentially a reflecting random walk with second largest eigenvalue* $\cos(\pi/k)$ [5, p. 389]. *Then the chain* $T_0 = e^{\Delta}$ *has the second largest eigenvalue* $\exp(\cos(\pi/k) - 1) \approx \exp(-(\pi^2/2)/k^2)$. *On the other hand, the bound of Lemma* 2.1 *gives* $\gamma \geq |S|^{-2} = k^{-2}$, *so the second eigenvalue* $\exp(-\gamma) \leq \exp(-1/k^2)$, *which is not an unreasonable bound.*

For $\beta > 0$ and the objective function f, Theorem 3.1 says that a sufficient number of steps is $e^{\beta h} k^2 (k \mu_{\beta,\max}) \log(\varepsilon \sqrt{\mu_\beta(\mathbf{x})})$. The dependence of β on the desired $\delta > 0$ and $\varepsilon > 0$ is explained in Lemma 3.1 and requires some estimates of the moment generating function ϕ.

EXAMPLE 3.2. *Consider the knapsack problem* [11, p. 14] *with general increasing utility functions* $f_i : \mathbf{R}_+ \to \mathbf{R}_+, f_i(0) = 0$. *The problem is to maximize* $f_1(q_1) + \cdots + f_d(q_d)$, *where* q_i *represents a nonnegative integer quantity of object* i, *subject to the overall weight constraint* $\langle \mathbf{w}, \mathbf{q} \rangle \leq W$, *where* $\mathbf{w} = (w_1, \ldots, w_d)$ *is a vector of positive integer weights and* W *is a positive integer.*

Add a slack variable x_{d+1} so that its corresponding indeterminate ξ_{d+1} is less than ξ_d. This ordering is important to get a simple Gröbner basis. For $\mathbf{x} = (x_1, \ldots, x_d, x_{d+1}) \in Z_+^{d+1}$, let $f(\mathbf{x}) = -(f_1(x_1) + \cdots + f_d(x_d))$. Then the problem becomes one to minimize $f(\mathbf{x})$ over S, where $S \subset Z_+^{d+1}$ is defined by $w_1 x_1 + \cdots + w_d x_d + x_{d+1} = W$.

To apply Theorem 3.1, observe that $h = f_{\max} - f_{\min} = 0 + \max\{f_1(q_1) + \cdots + f_d(q_d)\} \leq \sum_{i=1}^d f_i(W/w_i)$. Also, $|S|$ is the coefficient on z^W in the generating function

$$g(z) = \frac{1}{1-z} \prod_{i=1}^{d} \frac{1}{1 - z^{w_i}},$$

which is easily computed and satisfies $|S| \leq (W + d)^d / d!$. By Schur's theorem [17, p. 90], $|S|$ is well approximated by $W^d/(d! w_1 \ldots w_d)$ when W is large compared to d.

That a set of d moves on S from a Gröbner basis is, in general, easy to describe. Each corresponds to incrementing a coordinate 1 through d by ± 1 and adjusting the slack variable accordingly to maintain the equation $w_1 x_1 + \cdots + w_d x_d + x_{d+1} = W$ (cf. Proposition 3.1).

Theorem 3.1 says that a sufficient number of steps for the uniform distribution ($\beta = 0$) is roughly $d|S|^2 \log(\varepsilon/\sqrt{|S|})$, or essentially $dW^{2d}/(d!^2 w_1^2 \ldots w_d^2)$, if we ignore the logarithm. For $\beta > 0$, the quantity is roughly $de^{\beta h} W^{3d} \log(\varepsilon)/(d!^3 w_1^3 \cdots w_d^3)$. This quantity is polynomial in W for fixed d but is not polynomial in both W and d. The Ibarra–Kim theorem [15, p. 262] indicates that when the objective function is linear, there exists a dynamic programming "approximation" algorithm that is polynomial in both d and W, which would in theory be superior. The annealing method has the advantage in terms of generality, since it can easily be applied with any objective function. Neither the annealing algorithm nor the exact dynamic programming approach is fully polynomial in all the parameters.

In general, inequality constraints such as in the knapsack problem can be treated quite simply. Consider the situation where a state space S_0 is the intersection of a finite number of half-spaces, say $S_0 = \{x \in Z_+^d : A\mathbf{x} \leq \mathbf{b}\}$, where $\mathbf{b} \in Z_+^r$ and the nonnegative integer matrix A of rank r is such that $|S_0| < \infty$. This includes the knapsack problem of Example 3.3. By adding r slack variables, S_0 is equivalent to a finite state space S in Z_+^{d+r} with equality constraints. For the algebra, we need r new indeterminates ψ_i, which we order $\xi_1 > \cdots > \xi_d > \psi_1 > \cdots > \psi_r$. A Gröbner basis for the appropriate ideal is the generating set $\{\xi_i - \Psi^{A(\mathbf{e}_i)}, 1 \leq i \leq d\}$, with $\mathbf{e}_i$ the basis element for $\mathbf{R}^d$, since the S-polynomials leave remainder 0 when divided by this set. These polynomials correspond to d moves given by incrementing or decrementing each of the original coordinates, chosen uniformly from the d choices, and adjusting the slack variables accordingly. This is then a special case of the Markov chain described in [2] for uniform generation within an arbitrary convex set of lattice points in Z^d.

A path between points $\mathbf{x}$ and $\mathbf{y}$ can be constructed by moving within S_0 along the edges of a d-dimensional rectangle as follows. Let $\mathbf{z} = \min\{\mathbf{x}, \mathbf{y}\}$, which belongs to S_0. Join $\mathbf{x}$ to $\mathbf{z}$ by decrementing the first coordinate, then the second, etc. Then join $\mathbf{y}$ to $\mathbf{z}$ in the same manner. The two segments form a path from $\mathbf{x}$ to $\mathbf{y}$ within S_0. This path can be somewhat shorter than the one that arises from the division algorithm. The number of steps in the path $p_{\mathbf{xy}}$ is $\Sigma_i |x_i - y_i| \leq 2 \max\{\Sigma_i u_i : \mathbf{u} \in S_0\}$. Let $a_i - 1$ bound the ith coordinate of elements in S_0, so $\max\{x_i : (x_1, \ldots, x_d) \in S_0\} \leq a_i - 1, i = 1, \ldots, d$.

PROPOSITION 3.1. *Let S_0 be as above with $D = \max\{\Sigma_i x_i : \mathbf{x} \in S_0\}$, and let $A = \prod_{i=1}^d a_i$. Let T_β be the Markov transition operator on S_0 (or equivalently S) defined in* (2.1). *Then $\|T_\beta^n(\mathbf{x}, \cdot) - \mu_\beta\| \leq \varepsilon$ for all $n \geq -d2^{d+1} e^{\beta h} \mu_{\beta,\max} A D^2 \log(\varepsilon \sqrt{\mu_\beta(\mathbf{x})})$.*

Remark. When $\beta = 0, \mu_{\beta,\max} = |S|^{-1}$, so the bound is roughly

$$-d2^{d+1} D^2 (A/|S|) \log(\varepsilon/\sqrt{|S|})$$

for the uniform distribution. For a rectangular region A, $A/|S| = 1$, and this specializes to a quantity on the order of $d2^{d+1}D^2$. D measures the diameter of S_0 in the L^1 sense, so this is consistent with the results of [2], which suggest that for most convex regions in dimension d, the number of steps required is on the order of the squared diameter. The bounds of Theorem 3.1 and Proposition 3.1 are comparable when $|S|$ is comparable to D.

Proof. First we estimate the gap $\gamma = 1 - \lambda_2$ for K_β. With Proposition 1′ of [3], we see that $1/\gamma \leq \max_e Q(e)^{-1} \Sigma_{p_{\mathbf{xy}} \ni e} |p_{\mathbf{xy}}| \mu_\beta(\mathbf{x}) \mu_\beta(\mathbf{y})$, where $|p_{\mathbf{xy}}| \leq 2D$ denotes the number of edges in the path joining points $\mathbf{x}$ and $\mathbf{y}$. Now $Q(e)^{-1} \leq 2d/\mu_{\beta,\min}$. To bound $\Sigma_{p_{\mathbf{xy}} \ni e} 1$, consider the edge e joining vertices $\mathbf{u} = (u_1, u_2, \ldots, u_i, \ldots, u_d)$ and $\mathbf{u} - \mathbf{e}_i$ (here $\mathbf{e}_i$ is the ith basis element in $\mathbf{R}^d$). We need to count first all the ordered pairs $(\mathbf{x}, \mathbf{y}) \in S_0 \times S_0$ such that their connecting path can traverse e. Then half this number will bound the number of unordered pairs.

The edge e is either on the path from $\mathbf{x}$ down to $\mathbf{z} = \min\{\mathbf{x}, \mathbf{y}\}$ or from $\mathbf{y}$ down to $\mathbf{z}$. Since the ith coordinate is changed along the edge e, the coordinates $1, \ldots, i-1$ remain fixed throughout the remaining part of the path. Thus $u_j = \min\{x_j, y_j\}, j = 1, \ldots, i-1$. Also, since coordinates $i+1, \ldots, d$ have not yet been visited, $u_j = x_j$ for $j = i+1, \ldots, d$, or $u_j = y_j$ for $j = i+1, \ldots, d$, depending on whether the edge is in the segment from $\mathbf{x}$ to $\mathbf{z}$ or from $\mathbf{y}$ to $\mathbf{z}$.

Partition the pairs $(\mathbf{x}, \mathbf{y})$, whose connecting path goes through e into 2^{i-1} groups, where a group is identified with a sequence of 0's and 1's of length $i-1$, and a 0 in the jth place indicates $x_j \geq y_j$, whereas a 1 indicates $x_j < y_j, 1 \leq j \leq i-1$. Now the

size of each of these groups is at most $2a_1a_2\cdots a_{i-1}a_iDa_{i+1}\cdots a_d = 2AD$ as follows. For a particular sequence of 0's and 1's, the possible values of $(\mathbf{x},\mathbf{y})$ are constrained so that $x_j = u_j$ for indices $j \le i-1$ where there is a 1 (indicating $x_j < y_j$, and thus $x_j = \min(x_j, y_j) = u_j$), and similarly $y_j = u_j$ for indices $j \le i-1$ where there is a 0 (indicating $y_j \le x_j$, and thus $y_j = \min(x_j, y_j)$). For indices $i < j \le d$, either $(x_{i+1},\dots,x_d) = (u_{i+1},\dots,u_d)$ and the y coordinates are unclear, or $(y_{i+1},\dots,y_d) = (u_{i+1},\dots,u_d)$ and the x coordinates are unclear. Finally, the ith coordinates in both $\mathbf{x}$ and $\mathbf{y}$ can take at most a_i and also at most $\max\{x_i : \mathbf{x}\in S_0\}+1 \le D+1$ values, so the number of such pairs is at most $2(a_1a_2\cdots a_{i-1}\times a_iD\times a_{i+1}\cdots a_d)$.

Then summing over all 2^{i-1} groups and dividing by 2 to get unordered pairs $\{\mathbf{x},\mathbf{y}\}$ we get $\Sigma_{p_{\mathbf{xy}}\ni e}1 \le 2^{i-1}(2AD/2) \le 2^{d-1}AD$.

Therefore

$$1/\gamma \le (2d/\mu_{\beta,\min})\mu_{\beta,\max}^2 2D(2^{d-1}AD) = d\rho\mu_{\beta,\max}2^{d+1}AD^2 = d2^{d+1}e^{\beta h}\mu_{\beta,\max}AD^2.$$

Again using the basic bound $\|T_\beta^n(\mathbf{x},\cdot)-\mu_\beta\| \le 1/\sqrt{\mu_\beta(\mathbf{x})}\exp(-n\gamma)$, we see that $\|T_\beta^n(\mathbf{x},\cdot)-\mu_\beta\| \le \varepsilon$ for $n \ge -\log(\varepsilon\sqrt{\mu_\beta(\mathbf{x})})/\gamma$, which occurs if

$$n \ge -d2^{d+1}e^{\beta h}\mu_{\beta,\max}AD^2\log(\varepsilon\sqrt{\mu_\beta(\mathbf{x})}). \qquad \square$$

If we apply Proposition 3.1 to the knapsack problem of Example 3.2, we can let $a_i = (W/w_i)+1$. Then A is approximately the product $W^d/(w_1\cdots w_d)$, and the quantity $|S| \approx W^d/(d!w_1\dots w_d) \approx A/d!$ for W large and fixed d. Since $D \le W/\min_i w_i$, we get the estimate $d2^{d+1}W^2/(\min_i w_i)^2(A/|S|)$, or roughly the quantity $d2^{d+1}d!W^2/(\min_i w_i)^2$. For fixed d and weights w_i, this grows more slowly in W than the estimate $dW^{2d}/(d!^2w_1^2\dots w_d^2)$ from Example 3.2.

We mention finally that significant improvements are possible in situations where a certain block structure is present in the constraint set. Suppose that the constraint set $S \subset Z_+^d$ can be described by g independent constraints on disjoint sets of d_i variables, $1 \le i \le g$, as follows. Let $A_i : \mathbf{R}^{d_i} \to \mathbf{R}^{r_i}$ be a matrix with nonnegative integer entries which define a constraint set $S_i = \{\mathbf{x}\in Z_+^{d_i} : A_i(\mathbf{x}) = \mathbf{b}_i\}, i = 1,\dots,g$. Then we assume that S has the product form $S = S_1\times\cdots\times S_g$.

Let b_i index the start of the variables for constraint i, so $b_i = d_1+\cdots+d_{i-1}+1, i = 1,\dots,g$. Let M_i of size m_i be the set of moves corresponding to a Gröbner basis for the symmetric Markov chain on each of these sets S_i, $i = 1,\dots,g$, considered separately. Let K_i be the symmetric kernel on S_i given by

$$K_i(\mathbf{x},\mathbf{y}) = \frac{1}{2m_i} \qquad \text{if } \mathbf{y}\ge 0 \text{ and } \mathbf{y} = \mathbf{x}\pm f \text{ for some } f \text{ in } M_i, \tag{3.2}$$

and K_i vanishes otherwise. This means that one updates the d_i coordinates corresponding to the constraints A_i with moves from M_i. Take arbitrary positive weights $w_1,\dots,w_g$ with $w_1+\cdots+w_g = 1$, and form the irreducible kernel K on S by

$$K(h_1\otimes h_2\cdots\otimes h_g)(\mathbf{x}) = \sum_{i=1}^g w_ih_1\otimes\cdots\otimes K_i(h_i)\otimes\cdots\otimes h_g(\mathbf{x}), \tag{3.3}$$

which means that one chooses a block of coordinates i with probability w_i, and then one runs the chain K_i in S_i to update those d_i coordinates while leaving the others unchanged. The eigenvectors of K are the weighted averages of tensor products of

those for the kernels $\{K_i, i = 1, \ldots, g\}$, weighted by the family $\{w_i\}$, with eigenvalues being the corresponding weighted averages. It is then a simple fact that the gap γ for K, the difference between unity and the second largest eigenvalue, is $\gamma = \min\{w_i\gamma_i : i = 1, \ldots, g\}$, where γ_i is one minus the second largest eigenvalue for the kernel K_i on the set S_i. Below we consider a special case with uniform distribution on one-dimensional blocks.

EXAMPLE 3.3 (Reflecting random walk in a box [2]). *Consider the state space* $S_0 = \{\mathbf{x} \in Z_+^d : 0 \le x_i \le a - 1\}$ *for an integer* $a > 1$. *The reflecting random walk makes a transition from a lattice point by uniformly choosing one of the* $2d$ *neighbors and moving to the one selected if the candidate is within the box. The boundary points have some positive holding probability. Another description is that one uniformly chooses one of the* d *dimensions or coordinates to update, then one runs the one-dimensional reflecting random walk one step on that coordinate in the space* $\{0, 1, \ldots, a - 1\}$.

The state space S_0 is equivalent for our purposes to $S = \{\mathbf{x} \in Z_+^{2d} : x_{i,1} + x_{i,2} = a - 1, i = 1, \ldots, d\}$ by adding d slack variables. Applying Lemma 2.1 at this point to S yields a spectral estimate that is not accurate for $d \ge 2$. Recall that the exact gap $\gamma = (1 - \cos(\pi/a))/d \approx \pi^2/2a^2d$, which is on the order of the square of the euclidean diameter of S [2].

To get something comparable with our method, write $S = S_1 \times \cdots \times S_d$, where $S_i = \{\mathbf{x} \in Z_+^2 : x_{i,1} + x_{i,2} = a - 1\}$. The Markov chain on S_i is run with moves $M_i = \{(1, -1)\}$. With uniform weights $w_i = 1/d$, the kernel (3.3) is exactly the reflecting walk in the box, and Lemma 2.1 gives $\gamma_i \ge |S_i|^{-2} = a^{-2}$. Then K has gap at least $1/a^2d$ as the average of the kernels K_i, and this result is of the right size in the parameters a and d.

We conclude from this example that in situations where a product structure exists on the state space (and also on the objective function, which we have taken to be constant in this example) the bound of Lemma 2.1 can be significantly improved.

4. Conclusions. Nonnegative integer constraint sets are difficult and interesting domains for optimization and simulation problems. The results in this paper give general bounds on the time required for a given accuracy in some problems of simulation on such domains without prior enumeration of the state space. They are formulated in terms of computable quantities. In some interesting examples the bounds are quite accurate, in particular, when the state space S is low dimensional. An example where they would not be accurate would be simulation on the set of multigraphs with given vertex degrees, which can be interpreted as simulation on symmetric nonnegative integer matrices with certain row and column sums. Here the dimension is on the order of the number of vertices, and we would not expect the results to be useful in this case. The basic technique for estimating eigenvalues of Lemma 2.1 is generally not powerful in high dimensions (see [2]) but does not require detailed properties of the objective function f which appear in theoretical results on annealing. Furthermore, the techniques for estimating the spectral gap γ and the path length between two elements of the state space may be adapted in particular situations to yield substantial improvements. Examples of this are shown for inequality constraints and when a product structure exists on the constraint set.

Improving the bounds of this paper and extending them to the nonreversible annealing algorithms treated in somewhat abstract terms in [12] and [16] would serve as interesting problems for further related research.

REFERENCES

[1] O. Catoni, *Applications of sharp large deviations estimates to optimal cooling schedules*, Ann. Inst. H. Poincaré Probab. Statist., 27 (1991), pp. 463–518.

[2] P. Diaconis and L. Saloff-Coste, *Nash inequalities for finite Markov chains*, J. Theoret. Probab., 9 (1996), pp. 459–510.

[3] P. Diaconis and D. Stroock, *Geometric bounds for eigenvalues of Markov chains*, Ann. Appl. Probab., 1 (1991), pp. 36–61.

[4] P. Diaconis and B. Sturmfels, *Algebraic Algorithms for Sampling from Conditional Distributions*, Technical Report 6, Department of Statistics, Stanford University, Stanford, CA, 1993.

[5] W. Feller, *An Introduction to Probability Theory and Its Applications, Vol.* 1, 2nd ed., John Wiley, New York, 1957.

[6] S. Geman and D. Geman, *Stochastic relaxation, Gibbs distributions, and the Bayesian restoration of images*, IEEE Trans. Pattern Analysis and Machine Intelligence, 6 (1984), pp. 721–741.

[7] B. Gidas, *Nonstationary Markov chains and convergence of the annealing algorithm*, J. Stat. Phys., 39 (1985), pp. 73–131.

[8] B. Hajek, *Cooling schedules for optimal annealing*, Math. Oper. Res., 13 (1988), pp. 311–329.

[9] R. Holley and D. Stroock, *Simulated annealing via Sobolev inequalities*, Comm. Math. Phys., 115 (1988), pp. 553–569.

[10] S. Ingrassia, *On the rate of convergence of the Metropolis algorithm and Gibbs sampler by geometric bounds*, Ann. Appl. Probab., 4 (1994), pp. 347–389.

[11] E. L. Johnson, *Integer Programming: Facets, Subadditivity, and Duality for Group and Semigroup Problems*, CBMS-NSF Regional Conf. Ser. in Appl. Math., SIAM, Philadelphia, 1980.

[12] L. Miclo, *Remarques sur l'hypercontractivité et l'évolution de l'entropie pour des chaînes de Markov finies*, in Seminaire de Probabilités XXXI, J. Azéma, ed., Springer, New York, 1997, pp. 136–167.

[13] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C,* 2nd ed., Cambridge University Press, New York, 1992.

[14] B. Ripley, *Stochastic Simulation*, John Wiley, New York, 1987.

[15] A. Schrijver, *Theory of Linear and Integer Programming*, John Wiley, New York, 1986.

[16] A. Trouvé, *Rough large deviation estimates for the optimal convergence speed exponent of generalized simulated annealing algorithms*, Ann. Inst. H. Poincaré Probab. Statist., 32 (1996), pp. 299–348.

[17] H. Wilf, *Generating Functionology*, Academic Press, San Diego, 1988.